BINOMIAL EDGE IDEALS AND CONDITIONAL INDEPENDENCE STATEMENTS

JÜRGEN HERZOG, TAKAYUKI HIBI, FREYJA HREINSDÓTTIR, THOMAS KAHLE, AND JOHANNES RAUH

Abstract. We introduce binomial edge ideals attached to a simple graph G and study their algebraic properties. We characterize those graphs for which the quadratic generators form a Gröbner basis in a lexicographic order induced by a vertex labeling. Such graphs are chordal and claw-free. We give a reduced squarefree Gröbner basis for general G. It follows that all binomial edge ideals are radical ideals. Their minimal primes can be characterized by particular subsets of the vertices of G. We provide sufficient conditions for Cohen–Macaulayness for closed and nonclosed graphs.

Binomial edge ideals arise naturally in the study of conditional independence ideals. Our results apply for the class of conditional independence ideals where a fixed binary variable is independent of a collection of other variables, given the remaining ones. In this case the primary decomposition has a natural statistical interpretation.

Keywords: Binomial Ideals, Edge Ideals, Cohen–Macaulay rings, Conditional Independence Ideals, Robustness.

Introduction

Let G be a simple graph on the vertex set $[n] = \{1, \ldots, n\}$, that is to say, G has no loops and no multiple edges. Furthermore let K be a field and $S = K[x_1, \ldots, x_n, y_1, \ldots, y_n]$ be the polynomial ring in $2n$ variables. For $i < j$ we set $f_{ij} = x_i y_j - x_j y_i$. We define the *binomial edge* ideal $J_G \subset S$ of G as the ideal generated by the binomials $f_{ij} = x_i y_j - x_j y_i$ such that $i < j$ and $\{i, j\}$ is an edge of G. Note that if G has an isolated vertex i, and G' is the restriction of G to the vertex set $[n] \setminus \{i\}$, then $J_G = J_{G'}$.

The class of binomial edge ideals is a natural generalization of the ideal of 2-minors of a $2 \times n$-matrix of indeterminates. Indeed, the ideal of 2-minors of a $2 \times n$-matrix may be interpreted as the binomial edge ideal of a complete graph on $[n]$. Related to binomial edge ideals are the ideals of adjacent minors considered by Hoşten and Sullivant [9]. In the case of a line graph our binomial edge ideal may be interpreted as an ideal of adjacent minors. This particular class of binomial edge ideals has also been considered by Diaconis, Eisenbud and Sturmfels in [4] where they compute the primary decomposition of this ideal.

Binomial edge ideals, as they are defined in this paper, also arise in the study of conditional independence statements [5]. They generalize a class which has been studied by Fink [7].

Classically one studies edge ideals of a graph G which are generated by the monomials $x_i x_j$ where $\{i, j\}$ is an edge of G. The edge ideal of a graph has been introduced by Villarreal [12] where he studied the Cohen–Macaulay property of such ideals. The purpose of this paper is to study the algebraic properties of binomial edge ideals in terms of properties of the underlying graph. In Section 1 we consider the Gröbner basis of J_G with

respect to the lexicographic order induced by $x_1 > x_2 > \cdots > x_n > y_1 > y_2 > \cdots > y_n$. We show in Theorem 1.1 that J_G has a quadratic Gröbner basis if G is closed with respect to the given labeling. Being closed can be characterized by the associated acyclic directed graph G^* with arrows (i, j) whenever $\{i, j\}$ is an edge of G and $i < j$. We show in Proposition 1.4 that G is closed if and only if for any two distinct vertices i and j of G^*, all shortest paths from i to j are directed. In Proposition 1.6 we give a sufficient condition for a closed graph to have a Cohen–Macaulay binomial edge ideal. In Theorem 2.1 we compute explicitly the reduced Gröbner basis of J_G for any simple graph G. This is one of the main results of this paper. As a consequence we see that the initial ideal of J_G is squarefree which in turn implies that J_G is a reduced ideal. Of course, Theorem 1.1 is a simple consequence of Theorem 2.1. But as the proof of Theorem 1.1 is quite simple and as it leads to the concept of closed graphs, we decided to present Theorem 1.1 independent from Theorem 1.1.

Section 3 is devoted to the study of the minimal prime ideals of J_G. In Theorem 3.2 we write J_G as a finite intersection of prime ideals which allows us to compute the dimension of S/J_G. It turns out that if S/J_G is Cohen–Macaulay, then $\dim S/J_G = |V(G)| + c$, where c is the number of connected components of G. As a simple consequence of this, one sees that a circle of length n is unmixed or Cohen–Macaulay, if and only if $n = 3$. As a last result of Section 3 we identify in Corollary3.9 the minimal prime ideals of J_G. They are related to the cut-points of certain subgraphs of G.

In the last section we discuss applications to the study of conditional independence ideals. For a class of conditional independence statements, suitable to model a notion of robustness, the results in the prior sections show that the corresponding ideal is a radical ideal. Furthermore, the primary decomposition can be computed, which yields a classification and parametrization of the set of probability distributions which satisfy these statements.

Terai informed the authors that M. Ohtani [10] independently obtained similar results for this class of ideals.

1. Edge ideals with quadratic Gröbner bases and closed graphs

We first study the question when J_G has a quadratic Gröbner basis.

Theorem 1.1. *Let G be a simple graph on the vertex set $[n]$, and let $<$ be the lexicographic order on $S = K[x_1, \ldots, x_n, y_1, \ldots, y_n]$ induced by $x_1 > x_2 > \cdots > x_n > y_1 > y_2 > \cdots > y_n$. Then the following conditions are equivalent:*

- (a) *The generators f_{ij} of J_G form a quadratic Gröbner basis;*
- (b) *For all edges $\{i, j\}$ and $\{k, l\}$ with $i < j$ and $k < l$ one has $\{j, l\} \in E(G)$ if $i = k$, and $\{i, k\} \in E(G)$ if $j = l$.*

Proof. (a) $\Rightarrow$ (b): Suppose (b) is violated, say, $\{i, j\}$ and $\{i, k\}$ are edges with $i < j < k$, but $\{j, k\}$ is not an edge. Then $S(f_{ik}, f_{ij}) = y_i f_{jk}$ belongs to J_G, but none of the initial monomials of the quadratic generators of J_G divides $\text{in}_<(y_i f_{jk})$.

(b) $\Rightarrow$ (a): We apply Buchberger's criterion and show that all S-pairs $S(f_{ij}, f_{kl})$ reduce to 0. If $i \neq k$ and $j \neq l$, then $\text{in}_<(f_{ij})$ and $\text{in}_<(f_{kl})$ have no common factor. It is well

known that in this case $S(f_{ij}, f_{kl})$ reduces to zero. On the other hand, if $i = k$, we may assume that $l < j$. Then

$$S(f_{ij}, f_{il}) = y_i f_{lj}$$

is the standard expression of $S(f_{ij}, f_{il})$. Similarly, if $j = l$, we may assume that $i < k$. Then

$$S(f_{ij}, f_{kj}) = x_j f_{ik}$$

is the standard expression of $S(f_{ij}, f_{kj})$. In both cases the S-pair reduces to 0. $\square$

Condition (b) of Theorem 1.1 does not only depend on the isomorphism type of the graph, but also on the labeling of its vertices. For example the graph G with edges $\{1,2\}$, $\{2,3\}$, and the graph G' with edges $\{1,2\}$, $\{1,3\}$ are isomorphic, but G satisfies condition (b), while G' does not.

In fact, condition (b) is a condition of the *associated directed graph* G^* of G which is defined as follows: the ordered pair (i,j) is an arrow of G^* if $\{i,j\}$ is an edge of G with $i < j$. The directed graph G^* is *acyclic*, that is, it has no directed cycles. Therefore we call G^* also the associated acyclic directed graph of G.

An acyclic directed graph is also called an *acyclic digraph* or simply a *DAG*. Acyclic directed graphs constitute an important class of directed graphs and play an important role in the modeling of information flows in networks. Any acyclic directed graph arises in the same way as we obtained G^* from G. Indeed, one of the fundamental results on acyclic directed graphs G is that they admit an *acyclic ordering* of its vertices, that is, the vertices of G can be ordered $v_1, \ldots, v_r$ such that for every arrow (v_i, v_j) of G we have $i < j$, see for example [2, Proposition 1.4.3]. An acyclic directed graph usually has many different acyclic orderings. In [11, Corollary 1.3] Stanley expressed the number of possible acyclic orderings in terms of the chromatic polynomial of G.

We say that a graph G on $[n]$ is *closed with respect to the given labeling of the vertices*, if G satisfies condition (b) of Theorem 1.1, and we say that a graph G with vertex set $V(G) = \{v_1, \ldots, v_n\}$ is *closed*, if its vertices can be labeled by the integer $1, 2, \ldots, n$ such that for this labeling G is closed.

Proposition 1.2. *If G is closed, then G is chordal and has no induced subgraph consisting of three different edges e_1, e_2, e_3 with $e_1 \cap e_2 \cap e_3 \neq \emptyset$.*

Proof. Suppose G is not chordal, then G contains a cycle C of length > 3 with no chord. Let i be the vertex of C with $i < j$ for all $j \in V(C)$, and let $\{i,j\}$ and $\{i,k\}$ be the edges of C containing i. Then $i < j$ and $i < k$, but $\{j,k\} \notin E(G)$.

Since G is closed, any induced subgraph is closed as well. Suppose there exists an induced subgraph H with three different edges e_1, e_2, e_3 such that three different edges e_1, e_2, e_3 with $e_1 \cap e_2 \cap e_3 \neq \emptyset$. Then there exists i such that $e_1 \cap e_2 \cap e_3 = \{i\}$. Say, $e_1 = \{i,j\}$, $e_2 = \{i,k\}$ and $e_3 = \{i,l\}$. Then $i \neq \min\{i,j,k,l\}$, otherwise H is not closed. If $j < i$, then $k > i$ and $l > i$, since H is closed. But then $\{k,j\}$ must be an edge of H, a contradiction. $\square$

A graph with three different edges e_1, e_2, e_3 such that $e_1 \cap e_2 \cap e_3 \neq \emptyset$ is called a *claw*. Hence Proposition 1.2 says that a closed graph is a claw-free chordal graph.

Corollary 1.3. *A bipartite graph is closed if and only if it is a line.*

Proof. A bipartite graph has no odd cycles. Since a closed graph is chordal, and since a chordal graph has an odd cycle, unless it is a tree, a closed bipartite graph must be a tree. If the tree is not a line, then there exists an induced subgraph which is a claw. Thus a closed bipartite graph must be a line.

Conversely, if G is a line of length l, then G is closed for the labeling of the vertices such that $\{1,2\},\{2,3\},\ldots,\{l,l+1\}$ are the edges of G. □

The conditions for being a closed graph formulated in Proposition 1.2 are only sufficient. For example the graph with edges $\{a,b\}$, $\{b,c\}$, $\{a,c\}$, $\{a,x\}$,$\{b,y\}$ and $\{c,z\}$ is chordal without a claw, but is not closed.

In the following we give a characterization of graphs which are closed with respect to a given labeling. Let G be a graph, and let v and w be vertices of G. A *path* π from v to w is a sequence of vertices $v=v_0,v_1,\ldots,v_l=w$ such that each $\{v_i,v_{i+1}\}$ is an edge of the underlying graph. If G is directed, then the path π is called *directed*, if either (v_i,v_{i+1}) is an arrow for all i, or (v_{i+1},v_i) is an arrow for all i.

Proposition 1.4. *A graph G on $[n]$ is closed with respect to the given labeling, if and only if for any two vertices $i\neq j$ of associated directed graph G^*, all paths of shortest length from i to j are directed.*

Proof. Suppose all shortest paths from i to j in G^* are directed. Let (i,j) and (i,k) be two arrow with $j<k$. Then $\{j,i\},\{i,k\}$ is a path from j to k which is not directed. So it cannot be the shortest path. Hence there exists the arrow (j,k). Similarly it follows that if (i,k) and (j,k) are arrows of G^* with $i<j$, then there must exist the arrow (i,j) in G^*. This shows that G^* is closed.

Conversely, assume that G is closed. Then there exists a labeling such that G^* is closed. Let i and j be two distinct vertices and let P be path of shortest length from i to j. Suppose P is not directed. Then there there exists a subpath r,s,t of P such that (r,s), (t,s), or $(s,r),s(s,t)$ in G^*. In both cases we may assume that $r<t$. Then, since G^* is closed, it follows that (r,t) is an arrow in G^*. Replacing the subpath r,s,t by r,t, we obtain a shorter path from i to j, a contradiction. □

In Proposition 1.4 it is important to require that *all* paths of shortest length from i to j are directed in order to conclude that G^* is closed. Indeed, consider the graph G with edges $\{1,2\}$, $\{2,3\}$, $\{3,4\}$ and $\{1,4\}$. Then the path $2,3,4$ is directed, while $2,1,4$ is not directed. But both paths are shortest paths between 2 and 4.

Proposition 1.5. *Let G be a simple graph on $[n]$. Then there exists a unique minimal (with respect to inclusion of edges) graph $\bar{G}$ on $[n]$ whose associated acyclic graph is closed with respect to the given labeling and such that G is a subgraph of $\bar{G}$.*

Proof. Consider the set $\mathcal{C}$ of graphs on $[n]$ containing G and whose associated acyclic graph is closed. This set is not empty, because the complete graph on $[n]$ belongs to this set. Since the intersection of any two graphs in $\mathcal{C}$ belongs again to $\mathcal{C}$, the assertion follows, as desired. □

The unique minimal closed graph $\bar{G}$ containing G is called the *closure* of G.

One basic question is which of the binomial edge ideals are Cohen–Macaulay. For a graph G, this is the case if and only the binomial edge of each component is Cohen–Macaulay. Thus it is enough to consider connected graphs. A partial answer on the Cohen–Macaulayness of binomial edge ideals is given in

Proposition 1.6. *Let G be a connected graph on $[n]$ which is closed with respect to the given labeling. Suppose further that G satisfies the condition that whenever $\{i, j+1\}$ with $i < j$ and $\{j, k+1\}$ with $j < k$ are edges of G, then $\{i, k+1\}$ is an edge of G. Then S/J_G is Cohen–Macaulay.*

Proof. We will show that $S/\operatorname{in}_<(J_G)$ is Cohen–Macaulay. This will then imply that S/J_G is Cohen–Macaulay as well.

Since the associated acyclic directed graph is closed, it follows from Theorem 1.1 that $\operatorname{in}_<(J_G)$ is generated by the monomials x_iy_j with $\{i, j\} \in E(G)$ and $i < j$. Applying the automorphism $\varphi\colon S \to S$ which maps each x_i to x_i, and y_j to y_{j-1} for $j > 1$ and y_1 to y_n, $\operatorname{in}_<(J_G)$ is mapped to the ideal generated by all monomials x_iy_j with $\{i, j+1\} \in E(G)$. This ideal has all its generators in $S' = K[x_1, \ldots, x_{n-1}, y_1, \ldots, y_{n-1}]$. Let $I \subset S'$ be the ideal generated by these monomials. Then $S/\operatorname{in}_<(J_G)$ is Cohen–Macaulay if and only if S'/I is Cohen–Macaulay. Note that I is the edge ideal of the bipartite graph Γ on the vertex set $\{x_1, \ldots, x_{n-1}, y_1, \ldots, y_{n-1}\}$, and with $\{x_i, y_j\} \in E(\Gamma)$ if and only if $\{i, j+1\} \in E(G)$. In [8] the Cohen–Macaulay bipartite graphs are characterized as follows: Suppose the edges of the bipartite graph can be labeled such that

(i) $\{x_i, y_i\}$ are edges for $i = 1, \ldots, n$;
(ii) if $\{x_i, y_j\}$ is an edge, then $i \leq j$;
(iii) if $\{x_i, y_j\}$ and $\{x_j, y_k\}$ are edges, then $\{x_i, y_k\}$ is an edge.

Then the corresponding edge ideal is Cohen–Macaulay.

We are going to verify these conditions for our edge ideal. Condition (ii) is trivially satisfied, and condition (iii) is a consequence of our assumption that whenever $\{i, j+1\}$ with $i < j$ and $\{j, k+1\}$ with $j < k$ are edges of G, then $\{i, k+1\}$ is an edge of G.

For condition (i) we have to show that $\{i, i+1\} \in E(G)$ for all i. But this follows from Proposition 1.4 which says that all shortest paths from i to $i+1$ are oriented paths. If $i, i+1$ would not be a path, then a shortest path from i to $i+1$ could not be oriented. Thus $i, i+1$ is a path in G, and hence $\{i, i+1\} \in E(G)$. $\square$

Examples 1.7. (a) Any complete graph satisfies the conditions of Proposition 1.6, so that S/J_G is Cohen–Macaulay. But of course this is well known because in this case J_G is the ideal of 2-minors of a generic $2 \times n$-matrix.

(b) Any line graph with the natural order of the vertices satisfies conditions of Proposition 1.6. Actually J_G is a complete intersection in this case.

(c) There are many more graphs satisfying the conditions of Proposition 1.6. For example the graph with edges $\{1, 2\}$, $\{2, 3\}$ $\{1, 3\}$ and $\{3, 4\}$.

(d) Not all closed graphs satisfy the conditions of Proposition 1.6. Such an example is the graph with edges $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$, $\{1, 4\}$ and $\{3, 4\}$. For this graph we have that $\operatorname{in}_<(J_G)$ and J_G are not Cohen–Macaulay.

(e) A graph G need not be closed for S/J_G being Cohen–Macaulay. The graph given after Corollary 1.3 is such an example.

2. The reduced Gröbner basis of a binomial edge ideal

We now come to the main result of this paper. For this we need to introduce the following concept: let G be a simple graph on $[n]$, and let i and j be two vertices of G with $i < j$. A path $i = i_0, i_1, \ldots, i_r = j$ from i to j is called *admissible*, if

- (i) $i_k \neq i_\ell$ for $k \neq \ell$;
- (ii) for each $k = 1, \ldots, r-1$ one has either $i_k < i$ or $i_k > j$;
- (iii) for any proper subset $\{j_1, \ldots, j_s\}$ of $\{i_1, \ldots, i_{r-1}\}$, the sequence $i, j_1, \ldots, j_s, j$ is not a path.

Given an admissible path

$$\pi : i = i_0, i_1, \ldots, i_r = j$$

from i to j, where $i < j$, we associate the monomial

$$u_\pi = (\prod_{i_k > j} x_{i_k})(\prod_{i_\ell < i} y_{i_\ell}).$$

Theorem 2.1. *Let G be a simple graph on $[n]$. Let $<$ be the monomial order introduced in Theorem 1.1. Then the set of binomials*

$$\mathcal{G} = \bigcup_{i<j} \{\, u_\pi f_{ij} \ : \ \pi \text{ is an admissible path from } i \text{ to } j \,\}$$

is a reduced Gröbner basis of J_G.

Proof. We organize this proof as follows: In First Step, we prove that $\mathcal{G} \subset J_G$. Then, since $\mathcal{G}$ is a system of generators, in Second Step, we show that $\mathcal{G}$ is a Gröbner basis of J_G by using Buchberger's criterion. Finally, in Third Step, it is proved that $\mathcal{G}$ is reduced.

First Step. We show that, for each admissible path π from i to j, where $i < j$, the binomial $u_\pi f_{ij}$ belongs J_G. Let $\pi : i = i_0, i_1, \ldots, i_{r-1}, i_r = j$ be an admissible path in G. We proceed with induction on r. Clearly the assertion is true if $r = 1$. Let $r > 1$ and $A = \{i_k : i_k < i\}$ and $B = \{i_\ell : i_\ell > j\}$. One has either $A \neq \emptyset$ or $B \neq \emptyset$. If $A \neq \emptyset$, then we set $i_{k_0} = \max A$. If $B \neq \emptyset$, then we set $i_{\ell_0} = \min B$.

Suppose $A \neq \emptyset$. It then follows that each of the paths $\pi_1 : i_{k_0}, i_{k_0-1}, \ldots, i_1, i_0 = i$ and $\pi_2 : i_{k_0}, i_{k_0+1}, \ldots, i_{r-1}, i_r = j$ in G is admissible. Now, the induction hypothesis guarantees that each of $u_{\pi_1} f_{i_{k_0},i}$ and $u_{\pi_2} f_{i_{k_0},j}$ belongs to J_G. A routine computation says that the S-polynomial $S(u_{\pi_1} f_{i_{k_0},i}, u_{\pi_2} f_{i_{k_0},j})$ is equal to $u_\pi f_{ij}$. Hence $u_\pi f_{ij} \in J_G$, as desired.

When $B \neq \emptyset$, the same argument as in the case $A \neq \emptyset$ is valid.

Second Step. It will be proven that the set of those binomials $u_\pi f_{ij}$, where π is an admissible path from i to j, forms a Gröbner basis of J_G. In order to show this we apply Buchberger's criterion, that is, we show that all S-pairs $S(u_\pi f_{ij}, u_\sigma f_{k\ell})$, where $i < j$ and $k < \ell$, reduce to zero. For this we will consider different cases.

In the case that $i = k$ and $j = \ell$, one has $S(u_\pi f_{ij}, u_\sigma f_{k\ell}) = 0$.

In the case that $\{i,j\} \cap \{k,\ell\} = \emptyset$, or $i = \ell$, or $k = j$, the initial monomials $\text{in}_<(f_{ij})$ and $\text{in}_<(f_{k\ell})$ form a regular sequence. Hence the S-pair $S(u_\pi f_{ij}, u_\sigma f_{k\ell})$ reduce to zero,

because of the following more general fact: let $f, g \in S$ such that $\mathrm{in}_<(f)$ and $\mathrm{in}_<(g)$ form a regular sequence and let u and v be any monomials. Then $S(uf, vg)$ reduces to zero.

It remains to consider the cases that either $i = k$ and $j \neq \ell$ or $i \neq k$ and $j = \ell$. Suppose we are in the first case. (The second case can be proved similarly.) We must show that $S(u_\pi f_{ij}, u_\sigma f_{i\ell})$ reduces to zero. We may assume that $j < \ell$, and must find a standard expression for $S(u_\pi f_{ij}, u_\sigma f_{i\ell})$ whose remainder is equal to zero.

Let $\pi : i = i_0, i_1, \ldots, i_r = j$ and $\sigma \colon i = i'_0, i'_1, \ldots, i'_s = \ell$. Then there exist unique indices a and b such that

$$i_a = i'_b \quad \text{and} \quad \{i_{a+1}, \ldots, i_r\} \cap \{i'_{b+1}, \ldots, i'_s\} = \emptyset.$$

Consider the path

$$\tau : j = i_r, i_{r-1}, \ldots, i_{a+1}, i_a = i'_b, i'_{b+1}, \ldots, i'_{s-1}, i'_s = \ell$$

from j to ℓ. To simplify the notation we write this path as

$$\tau \colon j = j_0, j_1, \ldots, j_t = \ell.$$

Let

$$j_{t(1)} = \min\{\, j_c \,:\, j_c > j,\ c = 1, \ldots, t \,\},$$

and

$$j_{t(2)} = \min\{\, j_c \,:\, j_c > j,\ c = t(1)+1, \ldots, t \,\}.$$

Continuing these procedures yield the integers

$$0 = t(0) < t(1) < \cdots < t(q-1) < t(q) = t.$$

It then follows that

$$j = j_{t(0)} < j_{t(1)} < \cdots < j_{t(q)-1} < j_{t(q)} = \ell$$

and, for each $1 \leq c \leq t$, the path

$$\tau_c : j_{t(c-1)}, j_{t(c-1)+1}, \ldots, j_{t(c)-1}, j_{t(c)}$$

is admissible.

The highlight of the proof is to show that

$$S(u_\pi f_{ij}, u_\sigma f_{i\ell}) = \sum_{c=1}^{q} v_{\tau_c} u_{\tau_c} f_{j_{t(c-1)} j_{t(c)}}$$

is a standard expression of $S(u_\pi f_{ij}, u_\sigma f_{i\ell})$ whose remainder is equal to 0, where each v_{τ_c} is the monomial defined as follows: Let $w = y_i \operatorname{lcm}(u_\pi, u_\sigma)$. Thus $S(u_\pi f_{ij}, u_\sigma f_{i\ell}) = -w f_{j\ell}$. Then

(i) if $c = 1$, then

$$v_{\tau_1} = \frac{x_\ell w}{u_{\tau_1} x_{j_{t(1)}}};$$

(ii) if $1 < c < q$, then

$$v_{\tau_c} = \frac{x_j x_\ell w}{u_{\tau_c} x_{j_{t(c-1)}} x_{j_{t(c)}}};$$

(iii) if $c = q$, then

$$v_{\tau_q} = \frac{x_j w}{u_{\tau_q} x_{j_{t(q-1)}}}.$$

Our work is to show that

$$wf_{j\ell} = \frac{wx_\ell}{x_{j_{t(1)}}} f_{jj_{t(1)}} + \sum_{c=2}^{q-1} \frac{wx_jx_\ell}{x_{j_{t(c-1)}}x_{j_{t(c)}}} f_{j_{t(c-1)}j_{t(c)}} + \frac{wx_j}{x_{j_{t(q-1)}}} f_{j_{t(q-1)}\ell}$$

is a standard expression of $wf_{j\ell}$ with remainder 0. In other words, we must prove that

$$(\sharp) \qquad w(x_jy_\ell - x_\ell y_j) \;=\; \frac{wx_\ell}{x_{j_{t(1)}}}(x_jy_{j_{t(1)}} - x_{j_{t(1)}}y_j) + \sum_{c=2}^{q-1} \frac{wx_jx_\ell}{x_{j_{t(c-1)}}x_{j_{t(c)}}}(x_{j_{t(c-1)}}y_{j_{t(c)}} - x_{j_{t(c)}}y_{j_{t(c-1)}}) + \frac{wx_j}{x_{j_{t(q-1)}}}(x_{j_{t(q-1)}}y_\ell - x_\ell y_{j_{t(q-1)}})$$

is a standard expression of $w(x_jy_\ell - x_\ell y_j)$ with remainder 0.

Since

$$wx_jy_\ell = \frac{wx_j}{x_{j_{t(q-1)}}} x_{j_{t(q-1)}}y_\ell > \frac{wx_jx_\ell}{x_{j_{t(q-2)}}x_{j_{t(q-1)}}} x_{j_{t(q-2)}}y_{j_{t(q-1)}} > \cdots > \frac{wx_jx_\ell}{x_{j_{t(1)}}x_{j_{t(2)}}} x_{j_{t(1)}}y_{j_{t(2)}} > \frac{wx_\ell}{x_{j_{t(1)}}} x_jy_{j_{t(1)}},$$

it follows that, if the equality $(\sharp)$ holds, then $(\sharp)$ turns out to be a standard expression of $w(x_jy_\ell - x_\ell y_j)$ with remainder 0. If we rewrite $(\sharp)$ as

$$w(x_jy_\ell - x_\ell y_j) = w(x_jx_\ell \frac{y_{j_{t(1)}}}{x_{j_{t(1)}}} - x_\ell y_j) + wx_jx_\ell \sum_{c=2}^{q-1} (\frac{y_{j_{t(c)}}}{x_{j_{t(c)}}} - \frac{y_{j_{t(c-1)}}}{x_{j_{t(c-1)}}}) + w(x_jy_\ell - x_jx_\ell \frac{y_{j_{t(q-1)}}}{x_{j_{t(q-1)}}}),$$

then clearly the equality holds.

Third Step. Finally, we show that the Gröbner basis $\mathcal{G}$ is reduced. Let $u_\pi f_{ij}$ and $u_\sigma f_{k\ell}$, where $i < j$ and $k < \ell$, belong to $\mathcal{G}$ with $u_\pi f_{ij} \neq u_\sigma f_{k\ell}$. Let $\pi : i = i_0, i_1, \ldots, i_r = j$ and $\sigma : k = k_0, k_1, \ldots, k_s = \ell$. Suppose that $u_\pi x_iy_j$ divides either $u_\sigma x_ky_\ell$ or $u_\sigma x_\ell y_k$. Then $\{i_0, i_1, \ldots, i_r\}$ is a proper subset of $\{k_0, k_1, \ldots, k_s\}$.

Let $i = k$ and $j = \ell$. Then $\{i_1, \ldots, i_{r-1}\}$ is a proper subset of $\{k_0, k_1, \ldots, k_s\}$ and $k, i_1, \ldots, i_{r-1}, \ell$ is an admissible path. This contradicts the fact that σ is an admissible path.

Let $i = k$ and $j \neq \ell$. Then y_j divide u_σ. Hence $j < k$. This contradicts $i < j$.

Let $\{i, j\} \cap \{k, \ell\} = \emptyset$. Then x_iy_j divide u_σ. Hence $i > \ell$ and $j < k$. This contradicts $i < j$. $\square$

Corollary 2.2. *J_G is a radical ideal.*

Proof. The assertion follows from Theorem 2.1 and the following general fact: let $I \subset S$ be a graded ideal with the property that $\mathrm{in}_<(I)$ is squarefree for some monomial order $<$. Then I is a radical ideal. Indeed, there exists an ideal $\tilde{I} \subset S[t]$ in the polynomial ring $S[t]$

such that t is a nonzerodivisor on $S[t]/\tilde{I}$ with $(S[t]/\tilde{I})/(tS[t]/\tilde{I}) \cong S/\operatorname{in}_<(I)$ and such that $\tilde{I}S[t,t^{-1}] = IS[t,t^{-1}]$, and there are positive degrees on the variables of $K[x_1,\ldots,x_n,t]$ such that $\tilde{I}$ is a graded ideal with respect to this grading. Thus we may apply the graded version of Lemma 4.4.9 in [3] in order to conclude that $\tilde{I}$ is a radical ideal. From the equality $\tilde{I}S[t,t^{-1}] = IS[t,t^{-1}]$, it follows that I is a radical ideal as well. $\square$

As a consequence of Theorem 2.1 we see that all admissible paths of a graph G can be determined by computing the reduced Gröbner basis of J_G.

On the other hand, it is not the case that for each edge $\{i,j\}$ in the closure of G there exists an admissible path from i to j. For example, for the graph G with edges $\{2,3\}$, $\{1,3\}$ and $\{1,4\}$, the edge $\{2,4\}$ belongs to the closure of G, but the only path $2,3,1,4$ from 2 to 4 is not admissible. Thus the reduced Gröbner basis of J_G does not give the closure of G.

3. The minimal prime ideals of a binomial edge ideal

Let G be a simple graph on $[n]$. For each subset $S \subset [n]$ we define a prime ideal P_S. Let $T = [n] \setminus S$, and let $G_1,\ldots,G_{c(S)}$ be the connected component of G_T. Here G_T is the *restriction* of G to T whose edges are exactly those edges $\{i,j\}$ of G for which $i,j \in T$. For each G_i we denote by $\tilde{G}_i$ the complete graph on the vertex set $V(G_i)$. We set

$$P_S(G) = (\bigcup_{i\in S}\{x_i,y_i\}, J_{\tilde{G}_1},\ldots,J_{\tilde{G}_{c(S)}}).$$

Obviously, $P_S(G)$ is a prime ideal. In fact, each $J_{\tilde{G}_i}$ is the ideal of 2-minors of a generic $2\times n_j$-matrix with $n_j = |V(G_j)|$. Since all the prime ideals $J_{\tilde{G}_j}$, as well as the prime ideal $(\bigcup_{i\in S}\{x_i,y_i\})$ are prime ideals in pairwise different sets of variables, $P_S(G)$ is a prime ideal, too.

Lemma 3.1. *With the notation introduced we have* $\operatorname{height} P_S(G) = |S| + (n - c(S))$.

Proof. We have

$$\begin{aligned}
\operatorname{height} P_S(G) &= \operatorname{height}(\bigcup_{i\in S}\{x_i,y_i\}) + \sum_{j=1}^{c(S)} \operatorname{height} J_{\tilde{G}_j} = 2|S| + \sum_{j=1}^{c(S)}(n_j - 1) \\
&= |S| + (|S| + \sum_{j=1}^{c(S)} n_j) - c(S) = |S| + (n - c(S)),
\end{aligned}$$

as required. $\square$

In [6] Eisenbud and Sturmfels showed that all associated prime ideals of a binomial ideal are binomial ideals. In our particular case we have

Theorem 3.2. *Let G be a simple graph on the vertex set $[n]$. Then* $J_G = \bigcap_{S\subset[n]} P_S(G)$.

Proof. It is obvious that each of the prime ideals $P_S(G)$ contains J_G. We will show by induction on n that each minimal prime ideal containing J_G is of the form $P_S(G)$ for some $S \subset [n]$. Since by Corollary 2.2, J_G is a radical ideal, and since a radical ideal is the intersection of its minimal prime ideals, the assertion of the theorem will follow.

We may assume that G is connected. Because if $G_1,\dots,G_r$ are the connected components of G, then each minimal prime ideal P of J_G is of the form $P_1+\dots+P_r$ where each P_i is a minimal prime ideal of J_{G_i}. Thus if each P_i has the expected form, then so does P. So now let G be connected and let P be a minimal prime ideal of J_G. Let T be the maximal subset of $\{x_1,\dots,x_n\}$ with the property that $T\subset P$ and that $x_i\in T$ implies $y_i\notin P$. We will show that $T=\emptyset$. This will then imply that if $x_i\in P$, then $y_i\in P$, as well.

We first observe that $T\neq\{x_1,\dots,x_n\}$. Because otherwise we would have $J_G\subset J_{\tilde{G}}\subsetneq (x_1,\dots,x_n)\subset P$, and P would not be a minimal prime ideal of J_G.

Suppose that $T\neq\emptyset$. Since $T\neq\{x_1,\dots,x_n\}$, and since G is connected there exists $\{i,j\}\in E(G)$ such that $x_i\in T$ but $x_j\notin T$. Since $x_iy_j-x_jy_i\in J_G\subset P$, and since $x_i\in P$ it follows that $x_jy_i\in P$. Hence since P is a prime ideal, we have $x_j\in P$ or $y_i\in P$. By the definition of T the second case cannot happen, and so $x_j\in P$. Since $x_j\notin T$, it follows that $y_j\in P$.

Let G' be the restriction of G to the vertex set to $[n]\setminus\{j\}$. Then

$$(J_{G'},x_j,y_j)=(J_G,x_j,y_j)\subset P.$$

Thus $\bar{P}=P/(x_j,y_j)$ is a minimal prime ideal of $J_{G'}$ with $x_i\in\bar{P}$ but $y_i\notin\bar{P}$ for all $x_i\in T\subset\bar{P}$. By induction hypothesis, $\bar{P}$ is of the form $P_S(G')$ for some subset $S\subset[n]\setminus\{j\}$. This contradicts the fact that $T\neq\emptyset$.

By what we have shown it follows that there exists a subset $S\subset[n]$ such that $P=(\bigcup_{i\in S}\{x_i,y_i\},\bar{P})$ where $\bar{P}$ is a prime ideal containing no variables. Let G' be the graph $G_{[n]\setminus S}$. Then reduction modulo the ideal $(\bigcup_{i\in S}\{x_i,y_i\})$ shows that $\bar{P}$ is a monomial prime ideal $J_{G'}$ which contains no variables. Let $G_1,\dots,G_c$ be the connected components of G'. We will show that $\bar{P}=(J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})$. This then implies that $P=(\bigcup_{i\in S}\{x_i,y_i\},J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})$, as desired.

To simplify notation we may as well assume that P contains no variables and have to show that $P=(J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})$, where $G_1,\dots,G_c$ are the connected components of G. In order to prove this we claim that if i,j with $i<j$ are two edges of G_k for some k, then $f_{ij}\in P$. From this it will then follow that $(J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})\subset P$. Since $(J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})$ is a prime ideal containing J_G, and P is a minimal prime ideal containing J_G, we conclude that $P=(J_{\tilde{G}_1},\dots,J_{\tilde{G}_c})$.

Let $i=i_0,i_1,\dots,i_r=j$ a path in G_k from i to j. We proceed by induction on r to show that $f_{ij}\in P$. The assertion is trivial for $r=1$. Suppose now that $r>1$. Our induction hypothesis says that $f_{i_1j}\in P$. On the other hand, one has $x_{i_1}f_{ij}=x_jf_{ii_1}+x_if_{i_1j}$. Thus $x_{i_1}f_{ij}\in P$. Since P is a prime ideal and since $x_{i_1}\notin P$, we see that $f_{ij}\in P$. $\square$

Lemma 3.1 and Theorem 3.2 yield the following

Corollary 3.3. *Let G be a simple graph on $[n]$. Then*

$$\dim S/J_G=\max\{(n-|S|)+c(S)\;:\;S\subset[n]\}.$$

In particular, $\dim S/J_G\geq n+c$, *where c is the number of connected components of G.*

In general, this inequality is strict. For example, for our claw G with edges $\{1,2\}$, $\{1,3\}$ and $\{1,4\}$ we have $\dim S/J_G=6$.

Corollary 3.4. *Let G be a simple graph on $[n]$ with c connected components. If S/J_G is Cohen–Macaulay, then* $\dim S/J_G = n + c$.

Proof. Since $P_\emptyset(G)$ does not contain any monomials, it follows that $P_S(G) \not\subseteq P_\emptyset(G)$ for any nonempty subset $S \subset [n]$. Thus Theorem 3.2 implies that $P_\emptyset(G)$ is a minimal prime ideal of J_G. Since $\dim S/P_\emptyset(G) = n + c$ and since S/J_G is equidimensional, the assertion follows. $\square$

Example 3.5. Consider the line graph G with n vertices. Then, as observed in Example 1.7, S/J_G is Cohen–Macaulay. It follows from Corollary 3.4 that $\dim S/P = n + 1$ for all minimal prime ideals of J_G. Let S be any subset of $[n]$. Then Theorem 3.2 and Corollary 3.3 imply that the minimal prime ideals of J_G are exactly those prime ideals $P_S(G)$ for which $c(S) = |S| + 1$. Let $S \subset [n]$. Then there exists integers $1 \leq a_1 \leq b_1 < a_2 \leq b_2 < a_3 \leq b_3 < \cdots < a_r \leq b_r \leq n$ such that

$$S = \bigcup_{i=1}^{r} [a_i, b_i] \quad \text{where for each } i, \quad [a_i, b_i] = \{j \in \mathbb{Z} \colon a_i \leq j \leq b_i\}.$$

We see that $|S| = \sum_{i=1}^r (b_i - a_i + 1) = \sum_{i=1}^r (a_i - b_i) + r$, and that

$$c(S) = \begin{cases} r - 1, & \text{if } a_1 = 1 \text{ and } b_r = n, \\ r, & \text{if } a_1 \neq 1 \text{ and } b_r = n, \text{ or } a_1 = 1 \text{ and } b_r \neq n, \\ r + 1, & \text{if } a_1 \neq 1 \text{ and } b_r \neq n. \end{cases}$$

Thus $c(S) = |S| + 1$ if and only if $a_1 \neq 1$, $b_r \neq n$ and $a_i = b_i$ for all i. In other words, the minimal prime ideals of G are those $P_S(G)$ for which S is a subset of $[n]$ of the form $\{a_1, a_2, \ldots, a_r\}$ with $1 < a_1 < a_2 < \ldots < a_r < n$. This is exactly the result of Diaconis, Eisenbud and Sturmfels [4, Theorem 4.3].

The question of when J_G is a prime ideal is easy to answer.

Proposition 3.6. *Let G be a simple graph on $[n]$. Then J_G is a prime ideal if and only if each connected component of G is a complete graph.*

Proof. Let $G_1, \ldots, G_r$ be the connected components of G, and suppose that J_G is a prime ideal. Since $P_\emptyset(G) = (J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_r})$ is a minimal prime ideal of J_G and J_G is a prime ideal, it follows that $J_G = (J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_r})$. On the other hand, $J_G = (J_{G_1}, \ldots, J_{G_r})$. Thus the desired conclusion is a consequence of the following observation. Suppose that G and G' are graphs on $[n]$ with $V(G) \subset V(G')$. Then $E(G) = E(G')$, if and only $J_G = J_{G'}$. $\square$

Corollary 3.7. *Let G be a cycle of length n. Then the following conditions are equivalent:*

(a) $n = 3$.
(b) *J_G is a prime ideal.*
(c) *J_G is unmixed.*
(d) *S/J_G is Cohen–Macaulay.*

Proof. Due to Proposition 3.6 the equivalence of (a) and (b) is clear, since a cycle of length n is a complete graph if and only if $n = 3$. It also follows from Proposition 3.6 that whenever J_G is a prime ideal, then J_G is Cohen–Macaulay, because if each of the components of G is a complete graph, then the binomial edge ideal of each component

is the ideal of 2-minors of a $2 \times k$-matrix for some k, and these ideals are known to be Cohen–Macaulay. Since J_G is unmixed if S/I_G is Cohen–Macaulay, all implications follow once it is shown that (c) implies (b). One of the minimal prime ideals of G is $P_\emptyset(G)$ and $\dim S/P_\emptyset(G) = n+1$. Now let $S \subset [n]$ with $S \neq \emptyset$. We may assume that we have labeled the edges of the cycle counterclockwise, and that

$$S = \bigcup_{i=1}^{r} [a_i, b_i] \quad \text{with} \quad 1 = a_1 \leq b_1 < a_2 \leq b_2 < \cdots a_r \leq b_r < n.$$

Then $c(S) = r$, and $\dim S/P_S(G) = n - |S| + c(S) = n - \sum_{i=1}^{r}(b_i - a_i) - r + r \leq n$. Thus if J_G is unmixed, then $P_\emptyset(G)$ is the only minimal prime ideal of J_G, and hence since J_G is reduced it follows that J_G is a prime ideal, as required. $\square$

Now let G be an arbitrary simple graph. Which of the ideals $P_S(G)$ are minimal prime ideals of J_G? The following result helps to find them.

Proposition 3.8. *Let G be a simple graph on $[n]$, and let S and T be subsets of $[n]$. Let $G_1, \ldots, G_s$ be the connected components of $G_{[n]\setminus S}$, and $H_1, \ldots, H_t$ the connected components of $G_{[n]\setminus T}$. Then $P_T(G) \subset P_S(G)$, if and only if $T \subset S$ and for all $i = 1, \ldots, t$ one has $V(H_i) \setminus S \subset V(G_j)$ for some j.*

Proof. For a subset $U \subset [n]$ we let L_U be the ideal generated by the variables $\{x_i, y_i \colon i \in U\}$. With this notation introduced we have $P_S(G) = (L_S, J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_s})$ and $P_T(G) = (L_T, J_{\tilde{H}_1}, \ldots, J_{\tilde{H}_t})$. Hence it follows that $P_T(G) \subset P_S(G)$, if and only if $T \subset S$ and $(L_S, J_{\tilde{H}_1}, \ldots, J_{\tilde{H}_t}) \subset (L_S, J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_s})$.

Observe that $(L_S, J_{\tilde{H}_1}, \ldots, J_{\tilde{H}_t}) = (L_S, J_{\tilde{H}'_1}, \ldots, J_{\tilde{H}'_t})$ where $H'_i = (H_i)_{[n]\setminus S}$. It follows that $P_T(G) \subset P_S(G)$ if and only if $(L_S, J_{\tilde{H}'_1}, \ldots, J_{\tilde{H}'_t}) \subset (L_S, J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_s})$ which is the case if and only if $(J_{\tilde{H}'_1}, \ldots, J_{\tilde{H}'_t}) \subset (J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_s})$, because the generators of the ideals $(J_{\tilde{H}'_1}, \ldots, J_{\tilde{H}'_t})$ and $(J_{\tilde{G}_1}, \ldots, J_{\tilde{G}_s})$ have no variables in common with the x_i and y_i for $i \in S$.

Since $V(Hi') = V(H_i) \setminus S$, the assertion will follow once we have shown the following claim: let $A_1, \ldots, A_s$ and $B_1, \ldots, B_t$ be pairwise disjoint subsets of $[n]$. Then

$$(J_{\tilde{A}_1}, \ldots, J_{\tilde{A}_s}) \subset (J_{\tilde{B}_1}, \ldots, J_{\tilde{B}_t}),$$

if and only if for each $i = 1, \ldots, s$ there exists a j such that $A_i \subset B_j$.

It is obvious that if the conditions on the A_i and B_j are satisfied, then we have the desired inclusion of the corresponding ideals.

Conversely, suppose that $(J_{\tilde{A}_1}, \ldots, J_{\tilde{A}_s}) \subset (J_{\tilde{B}_1}, \ldots, J_{\tilde{B}_t})$. Without loss of generality we may assume that $\bigcup_{j=1}^{t} B_j = [n]$. Consider the surjective K-algebra homomorphism

$$\varepsilon \colon S \to K[\{x_i, x_i z_1\}_{i \in B_1}, \ldots, \{x_i, x_i z_t\}_{i \in B_t}] \subset K[x_1, \ldots, x_n, z_1, \ldots, z_t]$$

with $\varepsilon(x_i) = x_i$ for all i and $\varepsilon(y_i) = x_i z_j$ for $i \in B_j$ and $j = 1, \ldots, t$. Then

$$\mathrm{Ker}(\varepsilon) = (J_{\tilde{B}_1}, \ldots, J_{\tilde{B}_t}).$$

Now fix one of the sets A_i and let $k \in A_i$. Then $k \in B_j$ for some k. We claim that $A_i \subset B_j$. Indeed, let $\ell \in A_i$ with $\ell \neq k$ and suppose that $\ell \in B_r$ with $r \neq j$. Since

$x_ky_\ell - x_\ell y_k \in J_{\tilde{A}_i} \subset (J_{\tilde{B}_1}, \dots, J_{\tilde{B}_t})$, it follows that $x_ky_\ell - x_\ell y_k \in \mathrm{Ker}(\varepsilon)$, so that $0 = \varepsilon(x_ky_\ell - x_\ell y_k) = x_kx_\ell z_j - x_kx_\ell z_r$, a contradiction. $\square$

Let $G_1, \dots, G_r$ be the connect components of G. Once we know the minimal prime ideals of J_{G_i} for each i the minimal prime ideals of J_G are known, Indeed, since the ideals J_{G_i} are ideals in different sets of variables, it follows that the minimal prime ideals of J_G are exactly the ideals $\sum_{i=t}^r P_i$ where each P_i is a minimal prime ideal of J_{G_i}.

The next results detects the minimal prime ideals of J_G when G is connected.

Corollary 3.9. *Let G be a connected simple graph on the vertex set $[n]$, and $S \subset [n]$. Then $P_S(G)$ is a minimal prime ideal of J_G if and only if $S = \emptyset$, or $S \neq \emptyset$ and for each $i \in S$ one has $c(S \setminus \{i\}) < c(S)$.*

In the terminology of graph theory, the corollary says that if G is a connected graph, then $P_S(G)$ is a minimal prime ideal of J_G, if and only if each $i \in S$ is a cut-point of the graph $G_{([n]\setminus S)\cup\{i\}}$.

Proof of 3.9. Assume that $P_S(G)$ is a minimal prime ideal of J_G. Let $G_1, \dots, G_r$ be the connected components of $G_{[n]\setminus S}$. We distinguish several cases.

Suppose that there is no edge $\{i,j\}$ of G such that $j \in G_k$ for some k. Set $T = S \setminus \{i\}$. Then the connected components of $G_{[n]\setminus T}$ are $G_1, \dots, G_r, \{i\}$. Thus $c(T) = c(S) + 1$. However this case cannot happen, since Proposition 3.8 would imply that $P_T(G) \subset P_S(G)$.

Next suppose that there exists exactly one G_k, say G_1, for which there exists $j \in G_1$ such that $\{i,j\}$ is an edge of G. Then the connected components of $G_{[n]\setminus T}$ are $G_1', G_2, \dots, G_r$ where $V(G_1') = V(G_1) \cup \{i\}$. Thus $c(T) = c(S)$. Again, this case cannot happen since Proposition 3.8 would imply that $P_T(G) \subset P_S(G)$.

It remains the case that there are at least two components, say $G_1, \dots, G_k$, $k \geq 2$, and $j_\ell \in G_\ell$ for $\ell = 1, \dots, k$ such that $\{i, j_\ell\}$ is an edge of G. Then the connected components of $G_{[n]\setminus T}$ are $G_1', G_{k+1}, \dots, G_r$, where $V(G_1') = \bigcup_{\ell=1}^k V(G_\ell) \cup \{i\}$. Hence in this case $c(T) < c(S)$.

Conversely, suppose that $c(S \setminus \{i\}) < c(S)$ for all $i \in S$. We want to show that $P_S(G)$. Suppose this is not the case. Then there exists a proper subset $T \subset S$ with $P_T(G) \subset P_S(G)$. We choose $i \in S \setminus T$. By assumption, we have $c(S \setminus \{i\}) < c(S)$. The discussion of the three cases above show that we may assume that $G_1', G_{k+1}, \dots, G_r$ are the components of $G_{\{}[n] \setminus \{i\})$ where $V(G_1') = \bigcup_{\ell=1}^k V(G_\ell) \cup \{i\}$ and where $k \geq 2$. It follows that $G_{[n]\setminus T}$ has one connected component H which contains G_1' Then $V(H) \setminus S$ contains the subsets $V(G_1)$ and $V(G_2)$. Hence $V(H) \setminus S$ is not contained in any $V(G_i)$. According to Proposition 3.8, this contradicts the assumption that $P_T(G) \subset P_S(G)$. $\square$

As an example of Corollary 3.9 consider again the cycle G of length n. Then, besides of the prime ideal $P_\emptyset(G)$ which is of height $n-1$, the only other minimal prime ideals are the ideals $P_S(G)$ where $|S| > 1$ and and no two elements $i, j \in S$ belong to the same edge of G. Each of these prime ideals has height n.

4. CI-Ideals

Binomial equations and determinantal ideals are of fundamental importance in the theory of conditional independence. In this final section we will demonstrate the connection between binomial edge ideals and conditional independence (CI) statements.

We consider a random vector $X = (X_0, \dots, X_N)$ of $N+1$ discrete random variables, where the random variable X_i takes values in the sets $[d_i]$ for some positive integers $d_i \in \mathbb{N}$. Then X takes values in $\mathcal{X} := [d_0] \times \cdots \times [d_N]$. A joint probability distribution of X is a non-negative real valued function $p : \mathcal{X} \to \mathbb{R}_{\geq 0}$, such that $\sum_{x \in \mathcal{X}} p(x) = 1$. It can be represented by a real vector $p = (p_{x_0,\dots,x_N})_{x_0,\dots,x_N} \in \mathbb{R}^{\mathcal{X}}$, where $p_{x_0,\dots,x_N}$ stands for the probability of the event $X_0 = x_0, X_1 = x_1, \dots, X_N = x_N$. In the following we will consider polynomial equations in these $\prod_{i=0}^{N} d_i$ indeterminates, denoting $\mathbb{C}[p_x : x \in \mathcal{X}]$ the ambient polynomial ring.

For any subset $S \subseteq \{0, \dots, N\}$ we write X_S for the collection of random variables $\{X_i : i \in S\}$. Then X_S is a random variable on the smaller state space $\mathcal{X}_S = \times_{i \in S}[d_i]$. Given $x_T \in \mathcal{X}_T$, we denote $\{X_T = x_T\} := \{y \in \mathcal{X} : y_i = x_i, \forall i \in T\}$. The notation $p(X_T = x_T) := \sum_{x \in \{X_T = x_T\}} p_x$ is common and convenient and may be abbreviated by $p(x_T)$, if no confusion can arise.

Let S and S' be two disjoint subsets of $\{0, \dots, N\}$, let $C \subseteq \mathcal{X}$, and fix a joint probability distribution p. We say that X_S is *conditionally independent* of $X_{S'}$ given C (under p) iff p satisfies all equations of the form

$$p(x_S, x_{S'}; C)p(x'_S, x'_{S'}; C) - p(x_S, x'_{S'}; C)p(x'_S, x_{S'}; C) = 0, \tag{1}$$

where $x_S, x'_S \in \mathcal{X}_S$, $x_{S'}, x'_{S'} \in \mathcal{X}_{S'}$, and

$$p(x_S, x_{S'}; C) := p(\{X_S = x_S\} \cap \{X_{S'} = X_{S'}\} \cap C) = \sum_{\substack{x \in C: \\ x(i) = x_S(i) \text{ for } i \in S, \\ x(i) = x_{S'}(i) \text{ for } i \in S'}} p_x \tag{2}$$

is the probability that X lies in C and agrees with x_S on S and with $x_{S'}$ on S'. In this case we write $X_S \perp\!\!\!\perp X_{S'} \,|C$. If $C = \mathcal{X}$, then it is customary to write $X_S \perp\!\!\!\perp X_{S'}$. Let $T \subseteq \{0, \dots, N\}$ be disjoint from S and S'. If $X_S \perp\!\!\!\perp X_{S'} \,|\{X_T = x_T\}$ holds for all $x_T \in \mathcal{X}_T$ we write $X_S \perp\!\!\!\perp X_{S'} \,|X_T$.

An ideal I which is generated by a collection of equations of the form (1) is called a *CI-ideal*. Here, equations (1) are seen as equations among the elementary probabilities p_x via the relations (2). Note that I is homogeneous. We can identify probability distributions satisfying the equations of I with those points of the projective variety of I which have real nonnegative homogeneous coordinates.

Example 4.1. Consider for a simple example $N = 2$ and binary variables $d_0 = d_1 = d_2 = 2$. The polynomial ring is given as $\mathbb{C}[p_{111}, p_{112}, p_{121}, p_{122}, p_{211}, p_{212}, p_{221}, p_{222}]$. The conditional independence $X_0 \perp\!\!\!\perp X_1 \,|X_2$ describes the binomial ideal

$$I_{X_0 \perp\!\!\!\perp X_1 \,|X_2} = (p_{111}p_{221} - p_{121}p_{211}, p_{112}p_{222} - p_{122}p_{212})$$

In contrast to that, the independence $X_0 \perp\!\!\!\perp X_1$ is given by the principal ideal

$$I_{X_0 \perp\!\!\!\perp X_1} = ((p_{111} + p_{112})(p_{221} + p_{222}) - (p_{211} + p_{212})(p_{121} + p_{122}))\,.$$

Remark 4.2. A conditional independence $X_S \perp\!\!\!\perp X_{S'}|C$ is usually defined differently: One requires

$$p(X_S = x_S, X_{S'} = x_{S'}|X \in C) = p(X_S = x_S|X \in C)p(X_{S'} = x_{S'}|X \in C) \tag{3}$$

for all $x_S \in \mathcal{X}_S$ and $x_{S'} \in \mathcal{X}_{S'}$. Here,

$$p(X_S = x_S, X_{S'} = y_{S'}|X \in C) = \frac{p(X_S = x_S, X_{S'} = y_{S'}, X \in C)}{p(X \in C)},$$

and so on. However, equation (3) is not well defined if $p(X \in C)$ is zero, while equation (1) is defined for all joint distributions p. It is an easy exercise to prove that equations (1) and (3) are equivalent if $p(X \in C)$ is nonzero.

We will now discuss a special case which makes it possible to apply the results of the first three sections. Namely, we assume $d_0 = 2$, i.e., X_0 is considered to be binary. In this case we can arrange the elementary probabilities p_x in a $2 \times d_1 \dots d_N$-matrix, where the columns are indexed by the state space $\mathcal{X}_{[N]}$ of $X_{[N]} = (X_1, \dots, X_N)$. The basic observation is that every 2-minor corresponds to one CI-statement; namely, the minor

$$p_{1x}p_{2x'} - p_{2x}p_{1x'}$$

of the two columns corresponding to $x, x' \in \mathcal{X}_{[N]}$ expresses exactly the CI-statement

$$X_0 \perp\!\!\!\perp X_{[N]} \,\big|\big\{X_{[N]} \in \{x, x'\}\big\} \,.$$

In this way we can associate a collection of CI-statements to every graph on the vertex set $\mathcal{X}_{[N]}$.

Until now we did not use of the fact that $X_{[N]}$ is a product of several random variables. Now let $S \cup T$ be a (disjoint) partition of $[N]$ and consider the CI-statement

$$X_0 \perp\!\!\!\perp X_S \,|X_T \,. \tag{4}$$

For simplicity we assume that $S = \{1, \dots, s\}$ for a moment. Then (4) is equivalent to the equations

$$p_{1x_Sx_T}p_{2x'_Sx_T} - p_{1x'_Sx_T}p_{2x_Sx_T}$$

for all $x_S, x'_S \in \mathcal{X}_S$ and $x_T \in \mathcal{X}_T$. These equations come from all 2-minors with columns $x, x' \in \mathcal{X}_{[N]}$ such that x and x' agree on their T-components. This means that we can associate with (4) the graph on $\mathcal{X}_{[N]}$ with edges

$$E(G) = \{(x, x') : \; x, x' \in \mathcal{X}_{[N]} \text{ agree on } T\}.$$

More generally, when we have a collection $\mathcal{C} = \{\, X_0 \perp\!\!\!\perp X_{S_i} \,|X_T \,\}$ of CI-statements corresponding to disjoint partitions $S_i \cup T_i$ of $[N]$, we can associate a graph G_i with every single statement. If we define a graph G on $\mathcal{X}_{[N]}$ by $E(G) = \bigcup_i E(G_i)$, then the binomial edge ideal of G equals the CI-ideal of $\mathcal{C}$.

CI-statements of the form under consideration have the following natural interpretation in probabilistic modeling: We consider X_0 as the output node of a system which receives input from $X_1, \dots, X_N$. Then we can ask how much information is lost when certain input nodes are not available. If $X_0 \perp\!\!\!\perp X_{S'} \,|X_T$, then all the relevant information can be reconstructed from X_T alone: The system can dispense with the information from $X_{S'}$. In this way, a collection of CI-statements can be used to model a notion of robustness of

probabilistic computation [1]. Because of this interpretation we introduce the following notation:

Definition 4.3. *A collection of CI-statements induced as above by a set of disjoint partitions $S_i \cup T_i = [N]$ will be called a* robustness specification*.*

Theorems 2.2 and 3.2 imply:

Corollary 4.4. *The CI-ideal of a robustness specification with binary output is a radical ideal.*

Now fix a robustness specification $\mathcal{C}$. Owing to Theorem 3.2, each minimal prime is given by a subset $S \subseteq \mathcal{X}_{[N]}$ which satisfies the conditions of Corollary 3.9. Such a subset S defines events with zero probability: $p(X_{[N]} \in S) = 0$ if $p \in V(P_S(G))$, where $G = G_{\mathcal{C}}$. In the language of statistical modeling, S is a set of structural zeros.

Corollary 4.5. *Let I be the CI-ideal of a robustness specification. Each minimal prime P of I is characterized by a set S of structural zeros in the distribution of $X_{[N]}$ which is common to all probability distributions lying in the component corresponding to P. The possible sets S are characterized by Corollary 3.9.*

The binomial generators $J_{\tilde{G}_1}, \dots, J_{\tilde{G}_{c(S)}}$ in $P_S(G)$ also have a nice statistical interpretation: Namely $J_{\tilde{G}_i}$ expresses the CI-statement

$$X_0 \perp\!\!\!\perp X_{[N]} \,\big|\, \big(X_{[N]} \in G_i\big) \,.$$

This means: If we know S, then the knowledge in which component of $G_{[N]\setminus S}$ the random vector $X_{[N]}$ lies contains all the relevant information about X_0. Once we know this component, the conditional probability distribution of X_0 is independent of any further information we may obtain. In other words, if we know G and S, then we can define a random variable C which maps every outcome of X with nonzero probability to the corresponding component in $[c(S)]$. We then have $X_0 \perp\!\!\!\perp X_{[N]} \,\big|\, C$, a fact which can be depicted by the following Markov chain

$$X_{[N]} \longrightarrow C \longrightarrow X_0.$$

This corresponds to the classical result that each irreducible component of a binomial ideal is essentially a toric variety [6], and in particular each irreducible component has a rational parametrization. The most natural such parametrization in the statistical setting is the following: p factors as a product of a distribution on the connected components $G_1, \dots, G_{c(S)}$ and a distribution of X_0 for each of the connected components. This should be compared to the dimension $n - |S| + c(S)$ in Lemma 3.3.

Each binomial ideal $I \subset \mathbb{C}[p_x : x \in \mathcal{X}]$ has the toric ideal $I : (\prod_{x \in \mathcal{X}} p_x)^\infty$ as a minimal prime. It corresponds to $S = \emptyset$, and all distributions with full support ($p(x) > 0$ for all $x \in \mathcal{X}$) satisfying the robustness specification are contained in the toric variety. We obtain the following

Corollary 4.6. *Let p be a probability distribution satisfying the robustness specification $\mathcal{C} = \{X_0 \perp\!\!\!\perp X_{S_i} \,|X_{T_i} \;:\; i = 1, \dots, r\}$. If p has full support (i.e., $p_x > 0$ for all $x \in \mathcal{X}$), then*

$$X_0 \perp\!\!\!\perp X_{\cup_i S_i} \,|X_{\cap_i T_i} \,.$$

In particular, if $\cup_i S_i = [N]$ *then* $X_0 \perp\!\!\!\perp X_{[N]}$ *and* X_0 *is unconditionally independent of the input.*

Remark 4.7. It is easy to prove this corollary directly using the *intersection axiom* [5].

This result is not surprising: If any combination of inputs in $\mathcal{X}_{[N]}$ is possible, then we can't deduce any missing information. Any distribution where X_0 is robust against perturbation of the inputs must make use of features of the input statistics.

Examples 4.8. Fix $k \in [N]$ and consider the collection of CI-statements

$$\left\{ X_0 \perp\!\!\!\perp X_S \,|X_T \ : S \in \binom{[N]}{k} \right\} \tag{5}$$

induced by all k-element subsets of $[N]$. Consider the graph G_k with vertices $\mathcal{X}_{[N]}$ and edges between any x and y which differ in at most k components. In other words, $\{x, y\} \in E(G_k)$ if and only if the *Hamming distance* between x and y is at most k. The CI-ideal for the statements (5) is the binomial edge ideal of G_k.
(a) If $k = 1$ and $d_i = 2$, for all $i \in [N]$ we find the graph of the N-cube.
(b) If $k = 1$ and $N = 2$ we have just two CI-statements:

$$X_0 \perp\!\!\!\perp X_1 \,|X_2 \ \text{ and } \ X_0 \perp\!\!\!\perp X_2 \,|X_1 \ .$$

These statements have been studied by A. Fink [7]. In this case the minimal primes can be seen to correspond to bipartite graphs Γ such that every connected component is a complete bipartite graph. The two groups of vertices in these graphs are $[d_1]$ and $[d_2]$. The corresponding prime is minimal if each vertex belongs to at least one edge. Such bipartite graphs are in bijection with pairs of partitions $[d_1] = I_1 \cup \cdots \cup I_c$ and $[d_2] = J_1 \cup \cdots \cup J_c$, where c is the number of connected components of Γ, and I_i resp. J_i are the vertices in the ith component of Γ. Then $S = \mathcal{X}_{[N]} \setminus \cup_{i=1}^{c}(I_i \times J_i)$ gives the link with our notation. In other words, the vertices of the connected components $G_1, \dots, G_{c(S)}$ are given by $V(G_i) = I_i \times J_i$.
(c) The considerations of (b) generalize to the case $k = N - 1$: As above, the minimal primes correspond to partitions $[d_i] = I_{i,1} \cup \cdots \cup I_{i,c}$, where $S = \mathcal{X}_{[N]} \setminus \cup_{j=1}^{c}(I_{1,j} \times \cdots \times I_{N,j})$, and the components of G_T satisfy $V(G_i) = I_{1,j} \times \cdots \times I_{N,j}$. We leave the verification of these results as an exercise to the reader. Unfortunately, the nice form of the connected components of G_T does not generalize for $k < N - 1$.

Acknowledgment

We wish to thank Seth Sullivant who established the contact between the two groups of authors. The last two authors thank Nihat Ay for pointing them at conditional independence problems in robustness theory.

References

[1] N. Ay and D.C. Krakauer, "Geometric Robustness Theory and Biological Networks," *Theory in Biosciences* **125** (2007), 93–121.
[2] J. Bang-Jensen and G. Gutin, "Digraphs: Theory, Algorithms and Applications," Springer, 2007.
[3] W. Bruns and J. Herzog, "Cohen–Macaulay rings," Revised Ed., Cambridge University Press, 1998.

[4] P. Diaconis, D. Eisenbud and B. Sturmfels, Lattice walks and primary decomposition, *in* "Mathematical Essays in Honor of Gian-Carlo Rota," Birkhäuser, Boston, Cambridge, MA, 1998, pp. 173–193.

[5] M. Drton, B. Sturmfels, S. Sullivant, "Lectures on Algebraic Statistics," Birkhäuser, 2009.

[6] D. Eisenbud and B. Sturmfels, Binomial ideals, *Duke Math. J.* **84** (1996), 1–45.

[7] Alex Fink, "The binomial ideal of the intersection axiom for conditional probabilities," preprint, arXiv:0902.1495.

[8] J. Herzog and T. Hibi, Distributive lattices, bipartite graphs and Alexander duality, *J. Algebraic Combin.* **22** (2005), 289–302.

[9] S. Hoşten and S. Sullivant, Ideals of adjacent minors, *J. Algebra* **277** (2004), 615–642.

[10] M. Ohtani, Graphs and Ideals generated by some 2-minors, to appear in Comm. Alg.

[11] R. Stanley, Acyclic orientations of graphs, *Discrete Math.* **5** (1973), 171–178.

[12] R. Villarreal, Cohen–Macaulay graphs, *Manuscripta Math.* **66** (1990), 277–293.

Jürgen Herzog, Fachbereich Mathematik, Universität Duisburg-Essen, Campus Essen, 45117 Essen, Germany

E-mail address: juergen.herzog@uni-essen.de

Takayuki Hibi, Department of Pure and Applied Mathematics, Graduate School of Information Science and Technology, Osaka University, Toyonaka, Osaka 560-0043, Japan

E-mail address: hibi@math.sci.osaka-u.ac.jp

Freyja Hreinsdóttir, School of Education, University of Iceland, Stakkahlid, 105 Reykjavik, Iceland

E-mail address: freyjah@hi.is

Thomas Kahle and Johannes Rauh, MPI for Mathematics in the Sciences, 04103, Leipzig, Germany

E-mail address: {kahle,rauh}@mis.mpg.de